

Bisphenol B  
77-40-7 | DTXSID4022442

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.69e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.52e-01

Confidence level: 4.38e-01

Nearest Neighbors from the Training Set

Image not found

3-Amino-3-(naphthalen-1-yl)propanoic acid

Measured: 2.57e-02  
Predicted: 1.36e-02

Image not found

Benzyl 4-hydroxyphenyl ketone

Measured: 3.16e-02  
Predicted: 6.55e-03

Image not found

1,3-Naphthalenediol

Measured: 1.12e-02  
Predicted: 2.01e-02